



*Fermilab*

*Accelerator Physics Center*

# Summary on “Modeling Radiation Effects in Magnets and Material Response”

Nikolai Mokhov

Fermilab

Workshop on Radiation Effects  
in Superconducting Magnet Materials

Fermilab

February 13-15, 2012

# Presentations

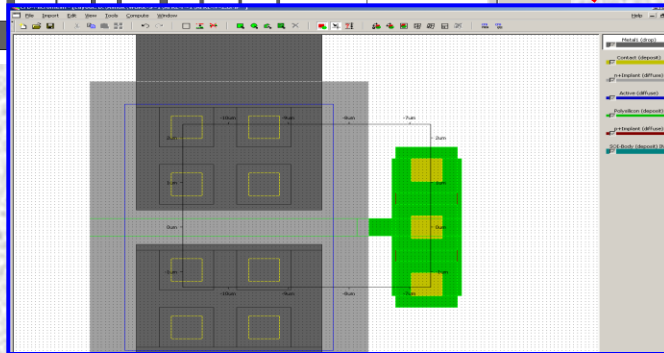
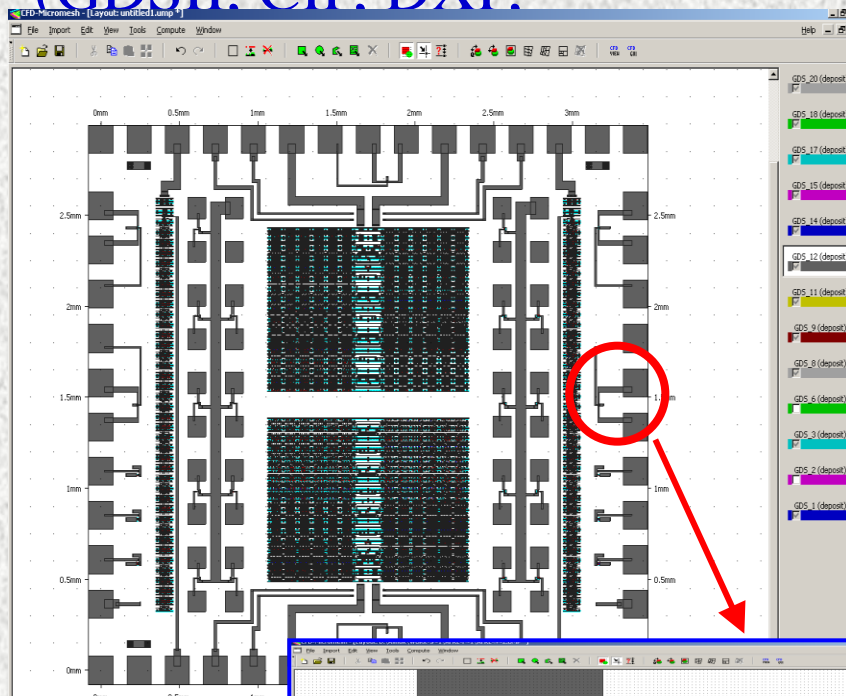
1. Marek Turowski and Alex Fedoseyev (CFDRC): Advanced tools for physics-based modeling of radiation effects
2. Nikolai Mokhov (FNAL): Radiation effect modeling: status, uncertainties and benchmarking needs
3. Igor Rakhno (FNAL): Improved description of ion stopping power in compounds
4. Yosuke Iwamoto (JAEA): Radiation damage calculation in PHITS over a wide energy range
5. Vitaly Pronskikh (FNAL): Radiation studies for Mu2e magnets
6. Reg Ronningen (MSU): Radiation environment and lifetime estimates for FRIB fragment separator superconducting magnets
7. Meimei Li (ANL): Moving from DPA to changes in materials properties



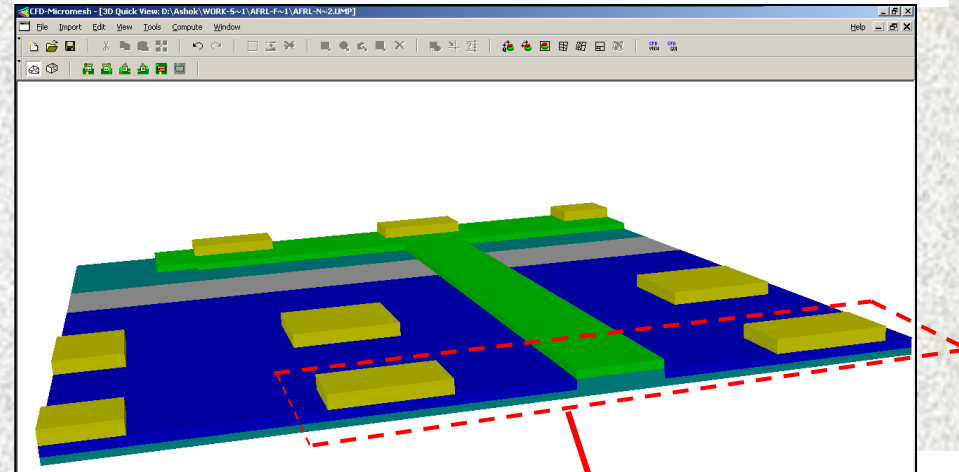
# CFDRC NanoTCAD

IC Layout → 3D Model → 3D Mesh → Simulation

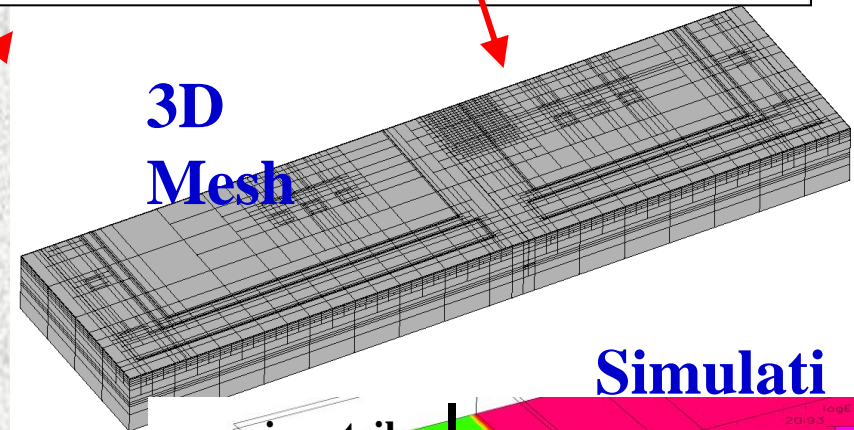
Imported Layout  
(GDSII, CIE, DXF)



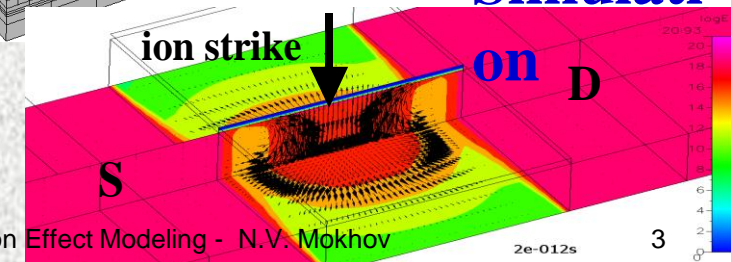
Automatic Generation of 3D



3D  
Mesh

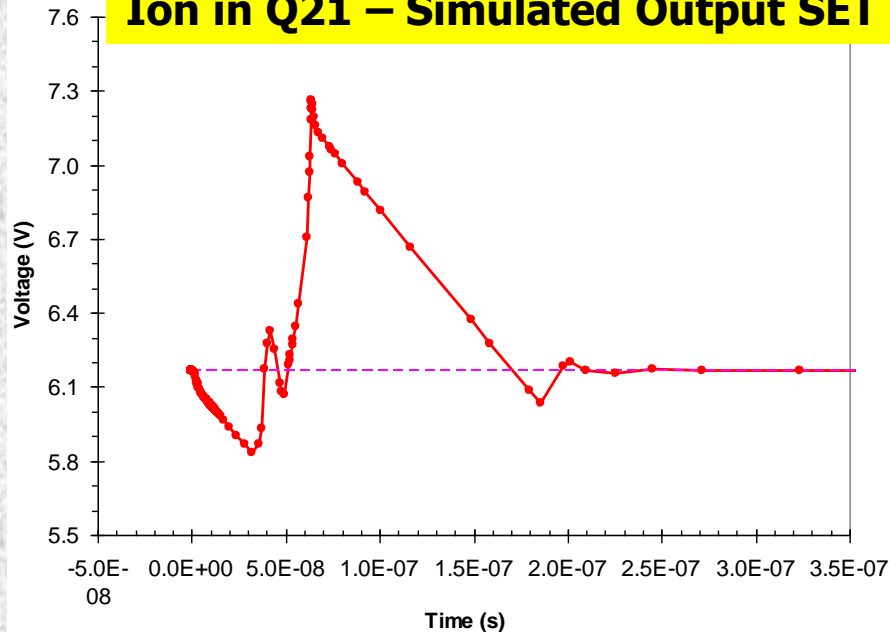


Simulati

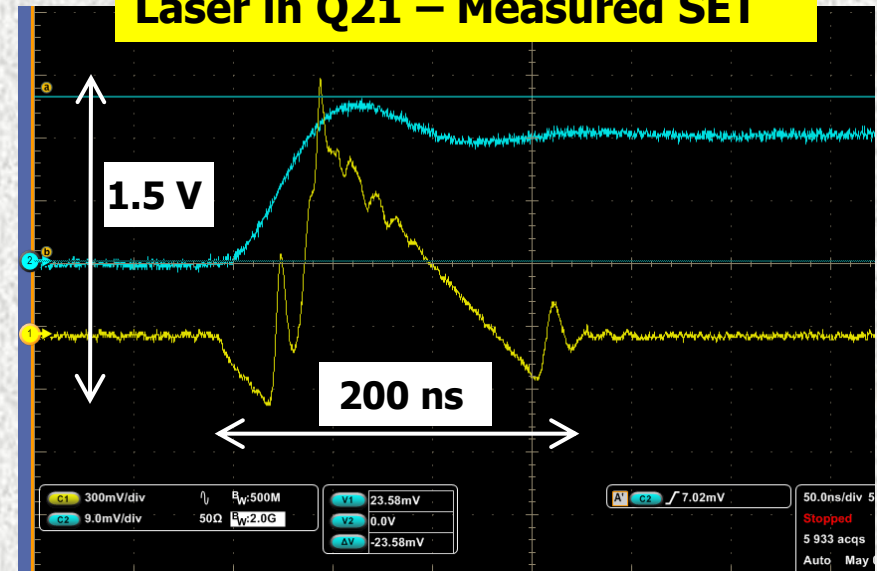


# CFDRC MixCad Simulations vs. Laser SEE Test Data

## Ion in Q21 – Simulated Output SET



## Laser in Q21 – Measured SET



**Excellent Agreement: both in SET Amplitude and Duration**

- CFDRC NanoTCAD / Mixed-Mode Tools validated !
- NG identified critical spots of the III-V Voltage Regulator design and is working on its radiation hardening.



# Subject and Issues

**What?** Primarily, production solenoids of Mu2e, COMET and Muon Collider ( $E_p = 1-15$  GeV), but also other superconducting setups in radiation fields

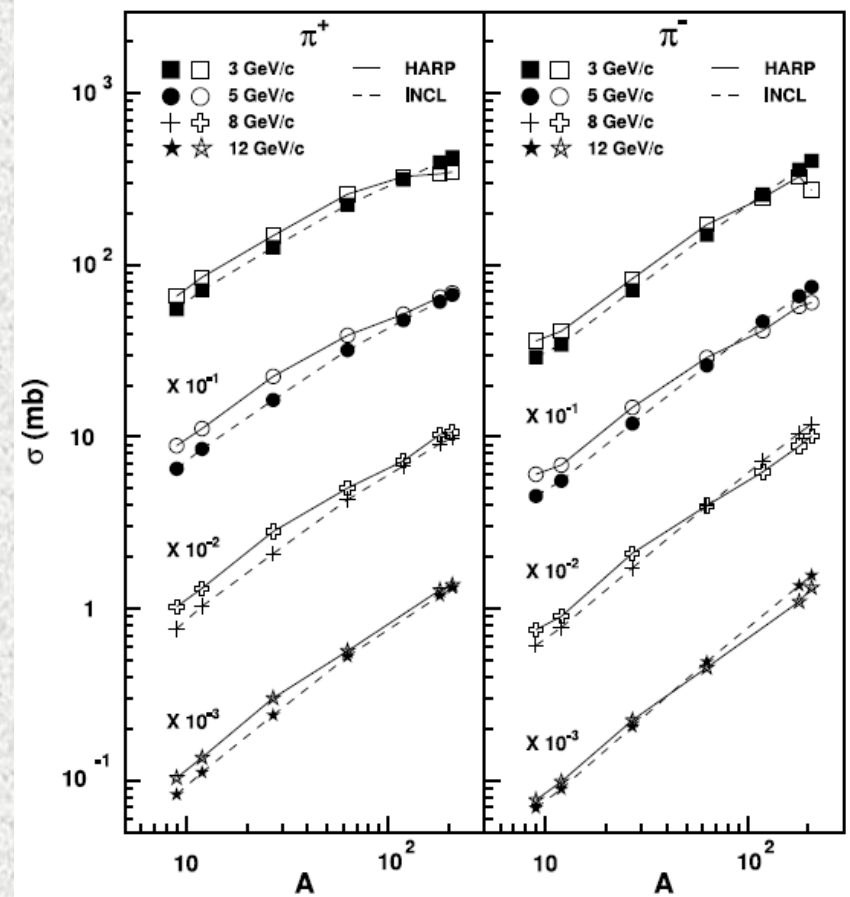
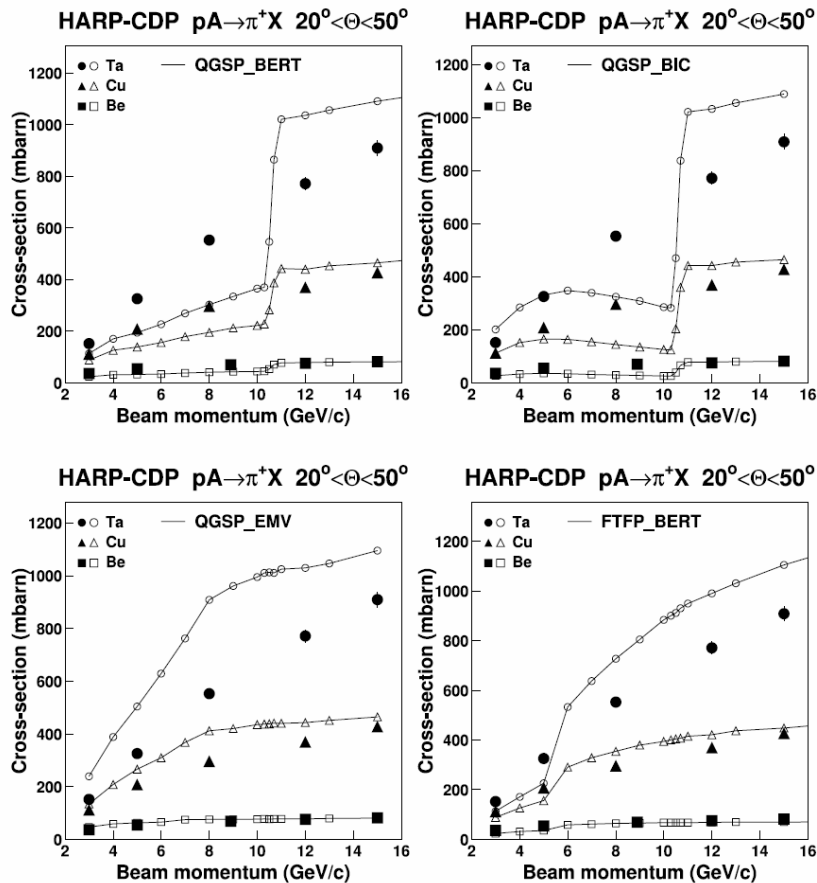
## Issues:

- Maximize useful particle & minimize background particle yields (also a primary source of all radiation effects considered here)
- Quench, integrity & lifetime: power density and integrated dose in critical components, e.g., SC coils, organic materials etc.
- Radiation damage to superconducting and stabilizing materials: DPA, helium gas production, integrated particle flux
- ES&H aspects: shielding, nuclide production, residual dose, impact on environment. Not forget electronics (SEU etc.)

Attacked via thorough simulations.

**How reliable are they?**

# Pion Production Cross-Sections at 3-15 GeV/c



3-15 GeV/c p on Be, Cu and Ta:  
GEANT4 models vs HARP

INCL-HE vs HARP

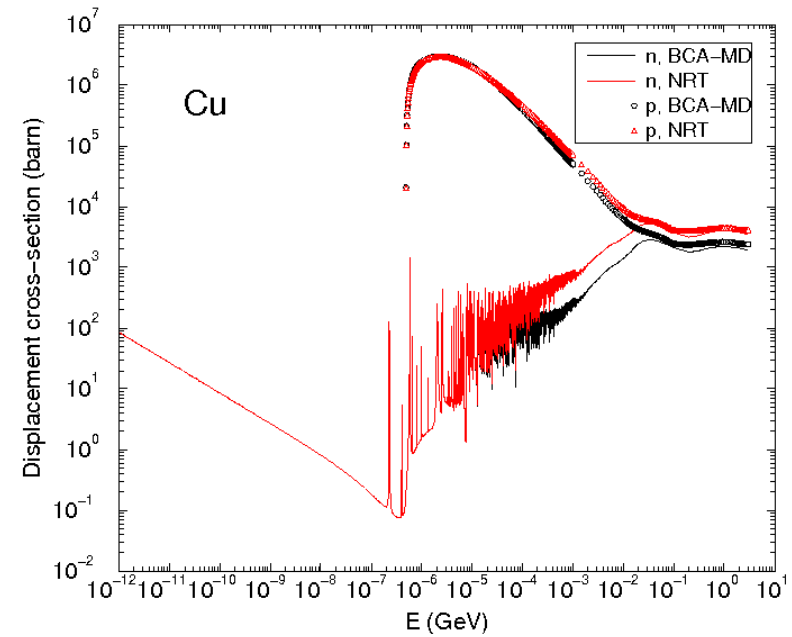
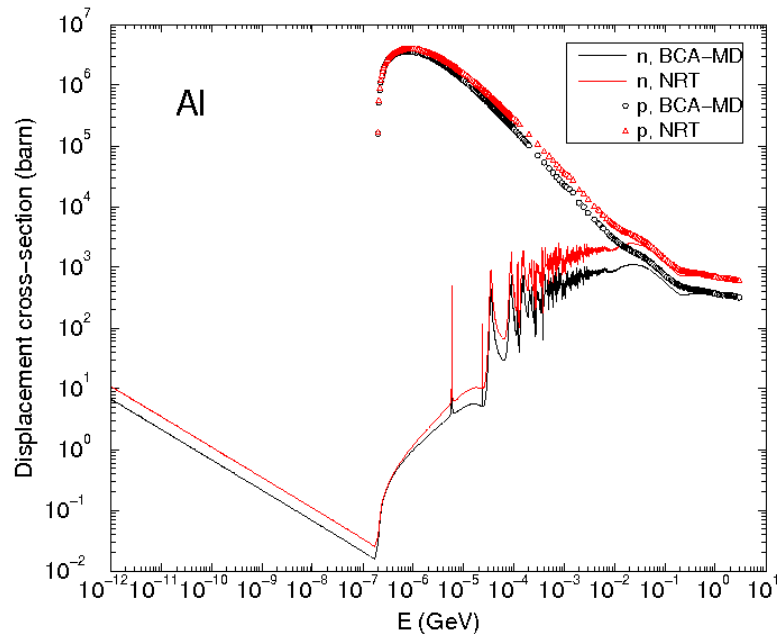
S. Pedoux, J. Cugnon



# Particle and Nuclide Production at 1-15 GeV: Status and Needs

- Production x-sections (total particle yields) modeled with the current versions of MARS15, FLUKA and INCL-HE agree within 10% with data. These code's event generators (for MARS15: CEM, LAQGSM and inclusive) predict general features of double differential x-sections, but can disagree with data up to a factor of 2 to 3 in some phase space regions. There are noticeably larger problems with GEANT4 models.
- Nuclide production is described quite reliably by the event generators of the above three codes, although there are issues with some channels.
- Models/Codes: model developments in transition region (2-7 GeV) and at  $E_p=1-30$  MeV; add PHITS predictions to the above benchmarking; more work on GEANT4.
- Data needs: low-energy pion/kaon/pbar spectra at  $E_p=2-7$  GeV; neutrons in fragmentation region; light fragment yields; nuclide yields for difficult cases; more ion and photon induced reactions.

# Nucleon Displacement x-section in Al and Cu



A. Konobeev

BCA-MD and pure NRT models can differ by a factor of two



# DPA and Radiation Damage: Status and Needs

- Modern models/codes which include Coulomb elastic scattering (crucial for high-Z projectiles), nuclear interactions, and same DPA model parameters agree quite well between each other and with (indirect) data. At the same time, industry standard NRT and state-of-the-art BCA-MD differ by a factor of 2 to 3 in some cases
- Models/codes: Strong dependencies on projectile type and energy (1 keV to a few GeV), projectile/target charge and nuclear form-factor and material properties to be further studied; work in progress in MARS on better low-energy neutron model; link DPA to changes in material properties
- Data needs: Annealed vs non-annealed defects; cryo temperatures!

# Stopping power in compounds

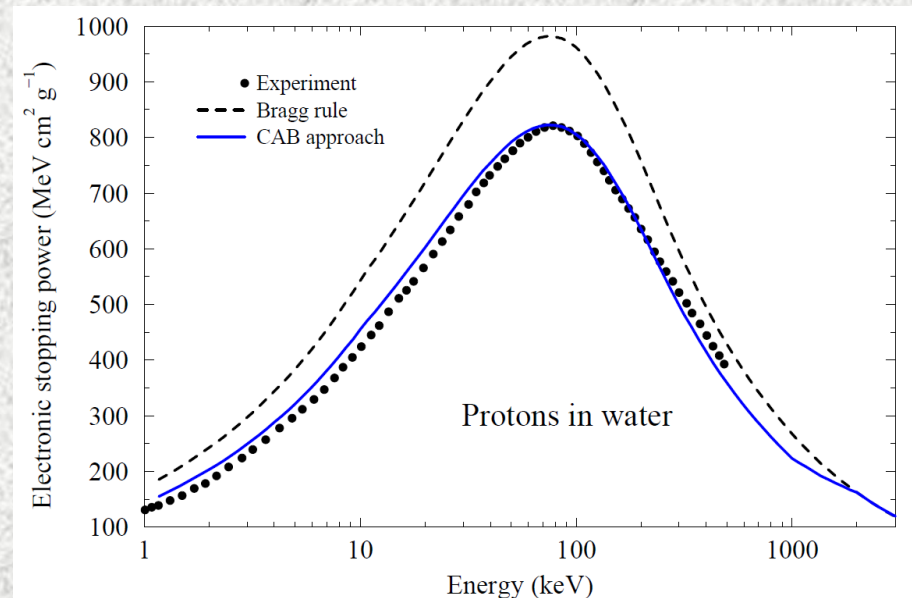
There is no need to invent the wheel: the *Cores-and-Bonds* approach (CAB) was developed in 80s by G. Both *et al.*, Köln University.

$$S_{\text{ion}} \xrightarrow{Z_{\text{eff}}} S_p \rightarrow S_{p,\text{Bragg}}, S_{p,\text{Bragg}}(125 \text{ keV}) \text{ and } S_{p,\text{CAB}}(125 \text{ keV})$$

$$S_{p,\text{CAB}}(125 \text{ keV}) = \sum \text{Cores} + \sum \text{Bonds}$$

Cores: **atoms** from H to Cl.

Bonds: **single** like H-H, C-H *etc*,  
**double** like C=C, C=O *etc*,  
**triple** like C≡C, O≡O.





# Radiation damage model in PHITS(3)

(1)Transport



(2) Energy transfer to target  
recoil atom with  
Coulomb scattering



(3) Cascade damage  
approximation

Improvement

$$\sigma_{\text{damage}} = \int_{t_d}^{t_{\text{max}}} \frac{d\sigma_{\text{scat.}}}{dt} \cdot \frac{0.8}{2 \cdot T_d} \underbrace{\frac{T}{1 + k_{\text{cascade}} \cdot g(\varepsilon)}}_{\text{Number of defects developed by NRT}} dt$$

Damage energy

M.J. Norgett, M.T. Robinson and I.M. Torrens: Nucl. Engineering and Design, 33, 50 (1975).

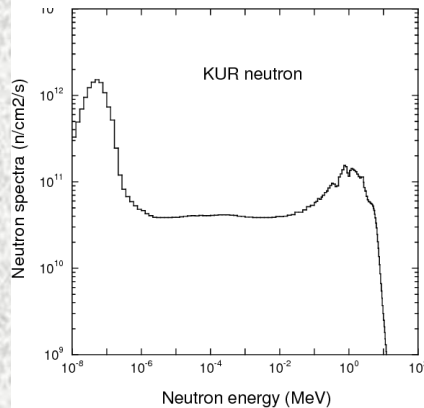
Integrating using dimensionless collision parameter  $t$

Number of defects developed by NRT

$T_d$ : the value of the threshold displacement energy. 30 eV for Cu and 90 eV for W

# Example of dpa calculation

## Calculation condition Reactor neutrons in Kyoto U.



target

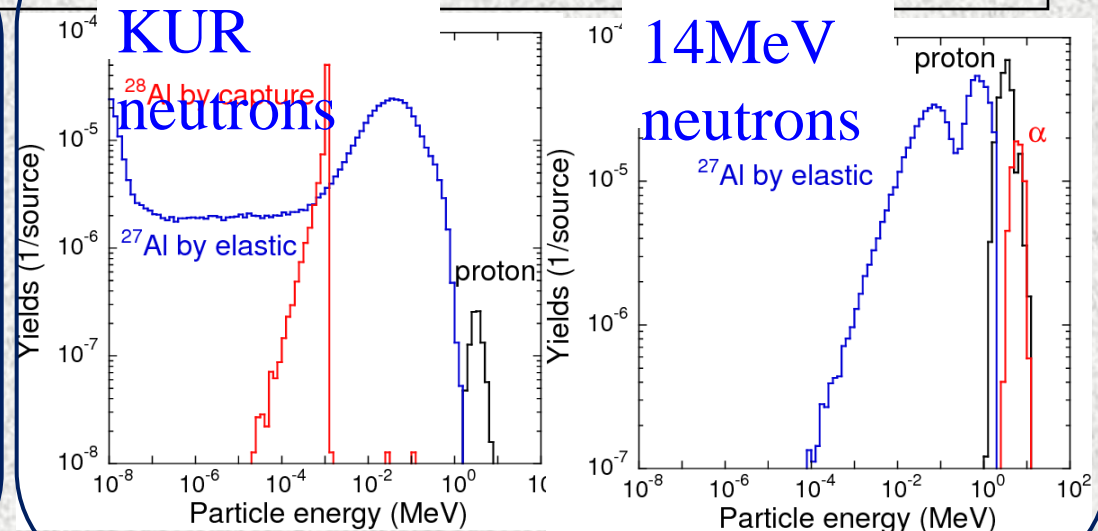
Al: 1mmx1mm  
x50mm



target

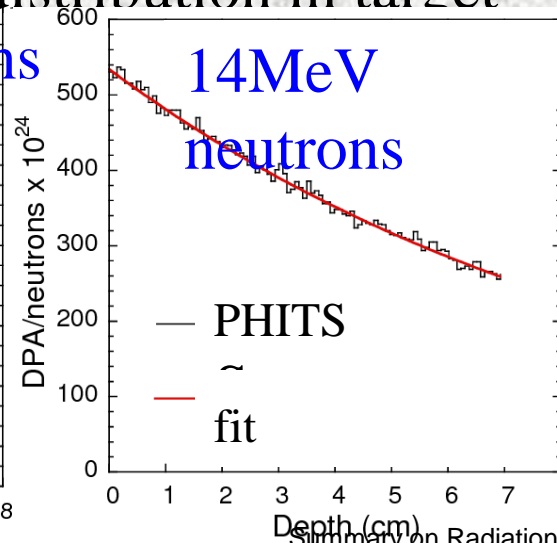
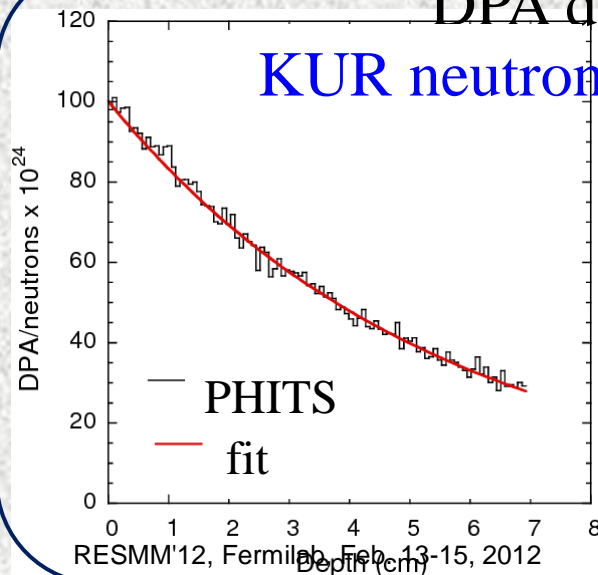
14MeV neutrons

## Particle production in target by PHITS



➤ Elastic scattering and capture are dominant.

## DPA distribution in target



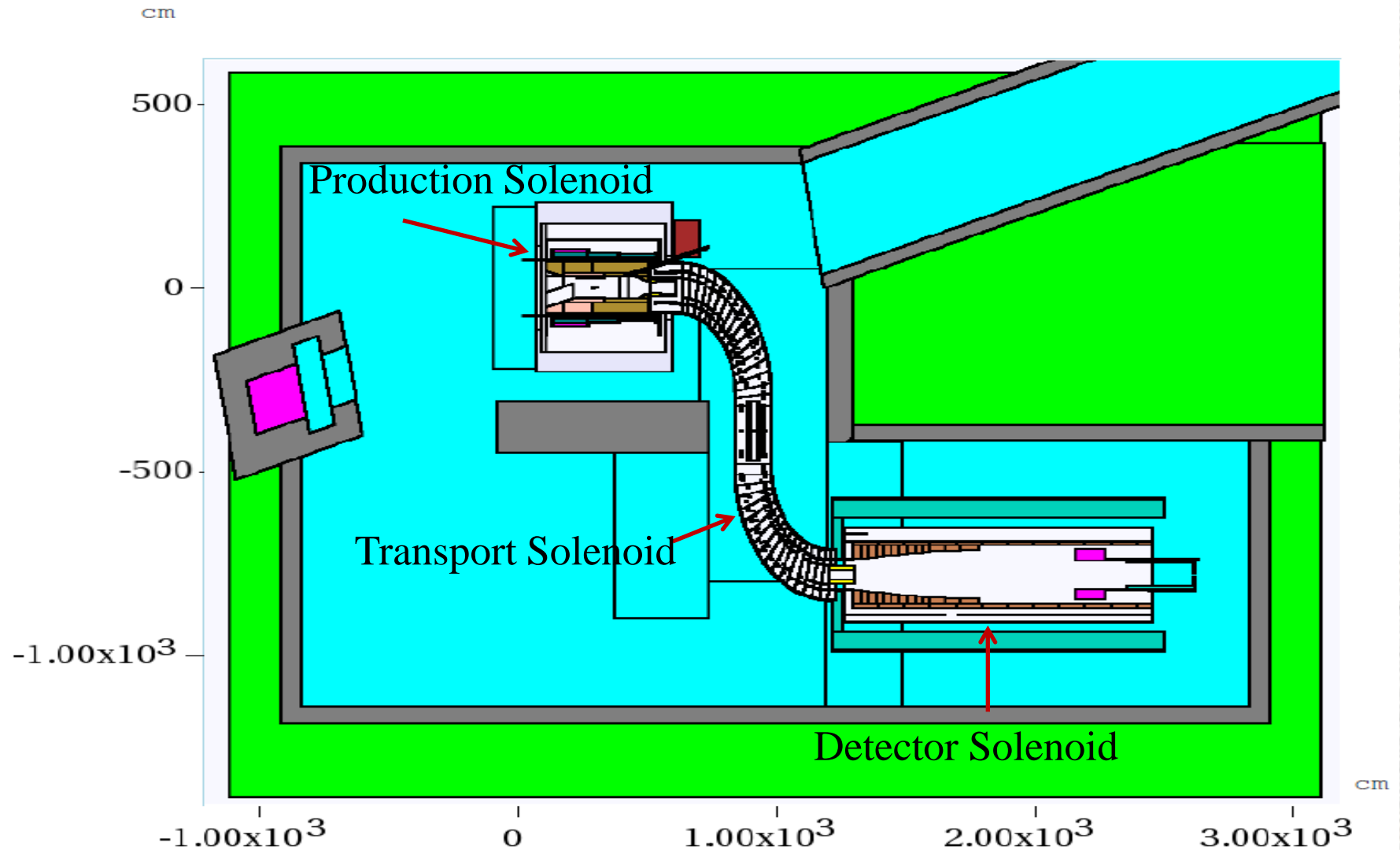
➤ PHITS can calculate detail dpa distribution in a target.

➤ SRIM code cannot calculate dpa for neutrons.

➤ DPA value decrease with depth, exponentially.



# Mu2e hall MARS15 model

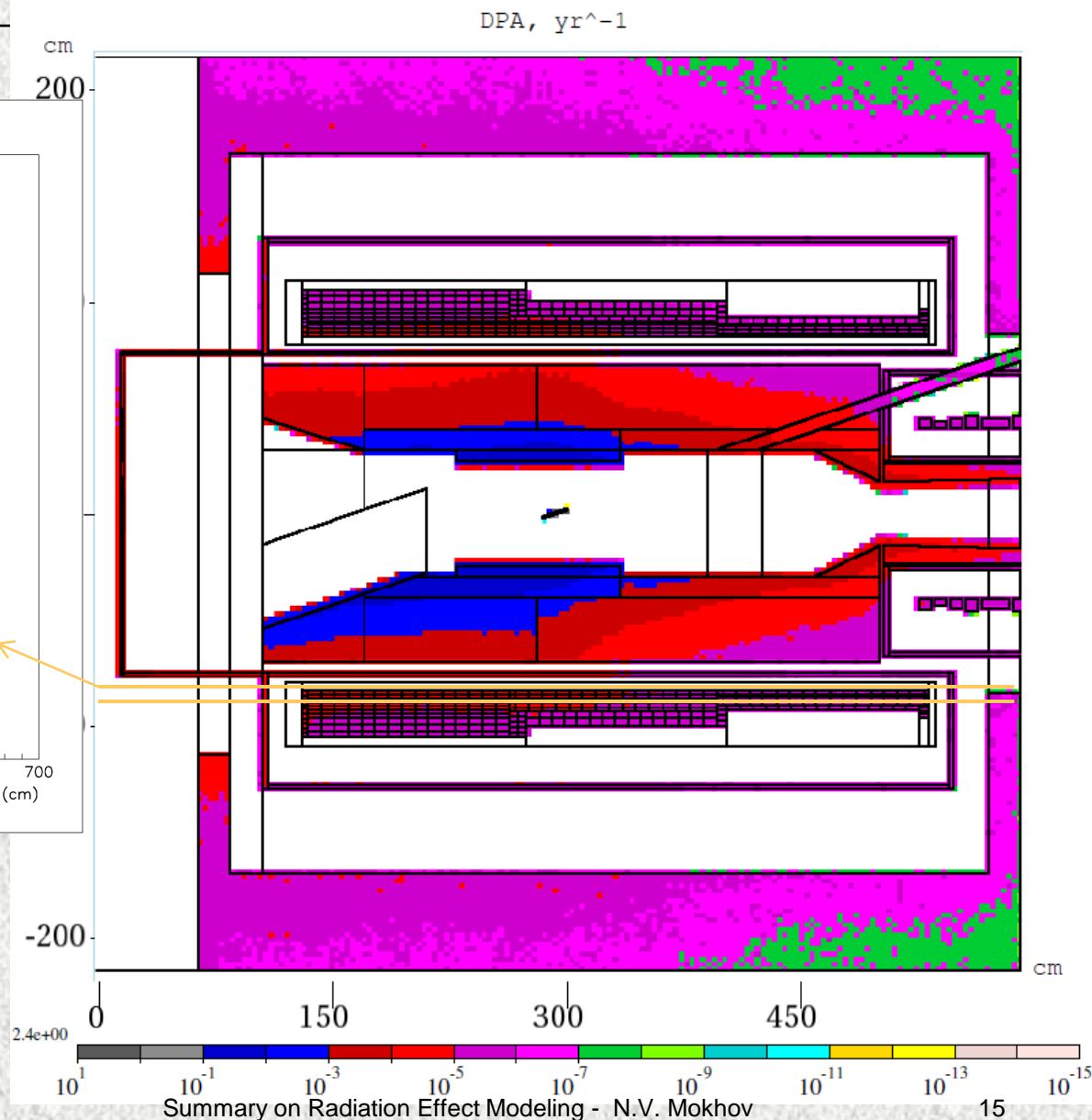
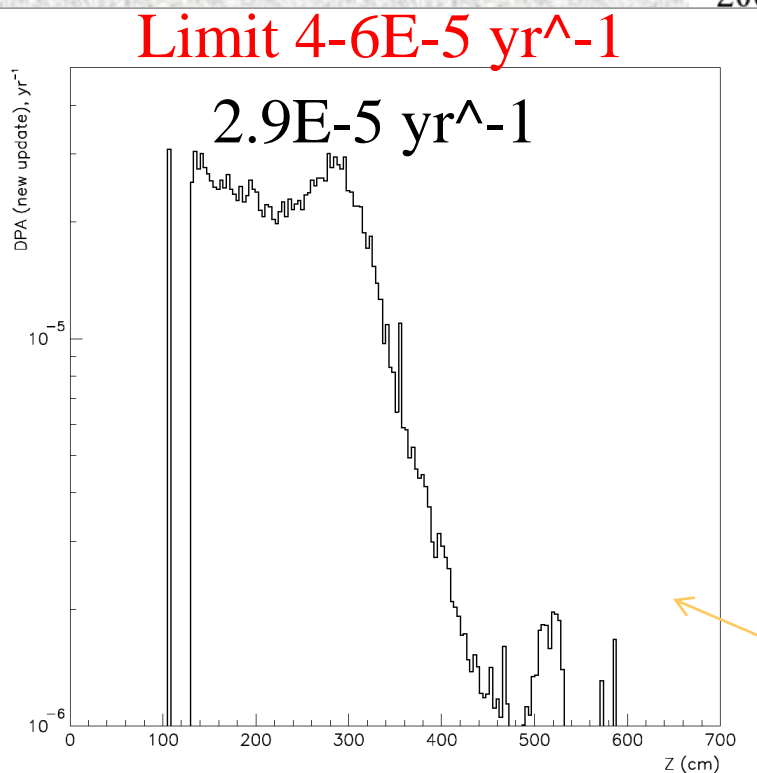


## Requirements to Heat and Radiation Shield

- Absorber (heat and radiation shield) is intended to prevent radiation damage to the magnet coil material and ensure quench protection and acceptable heat loads for the lifetime of the experiment
  - Total dynamic heat load on the coils (100 W)
  - Peak power density in the coils
  - Peak radiation dose to the insulation and epoxy
  - DPA to describe how radiation affects the electrical conductivity of metals in the superconducting cable

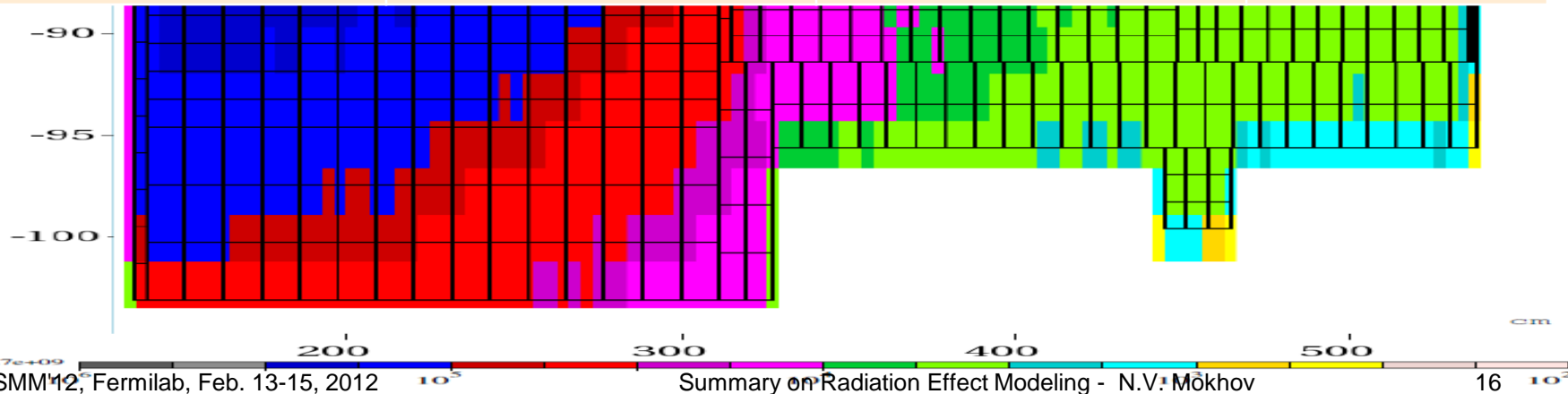


# DPA for nominal beam power baseline



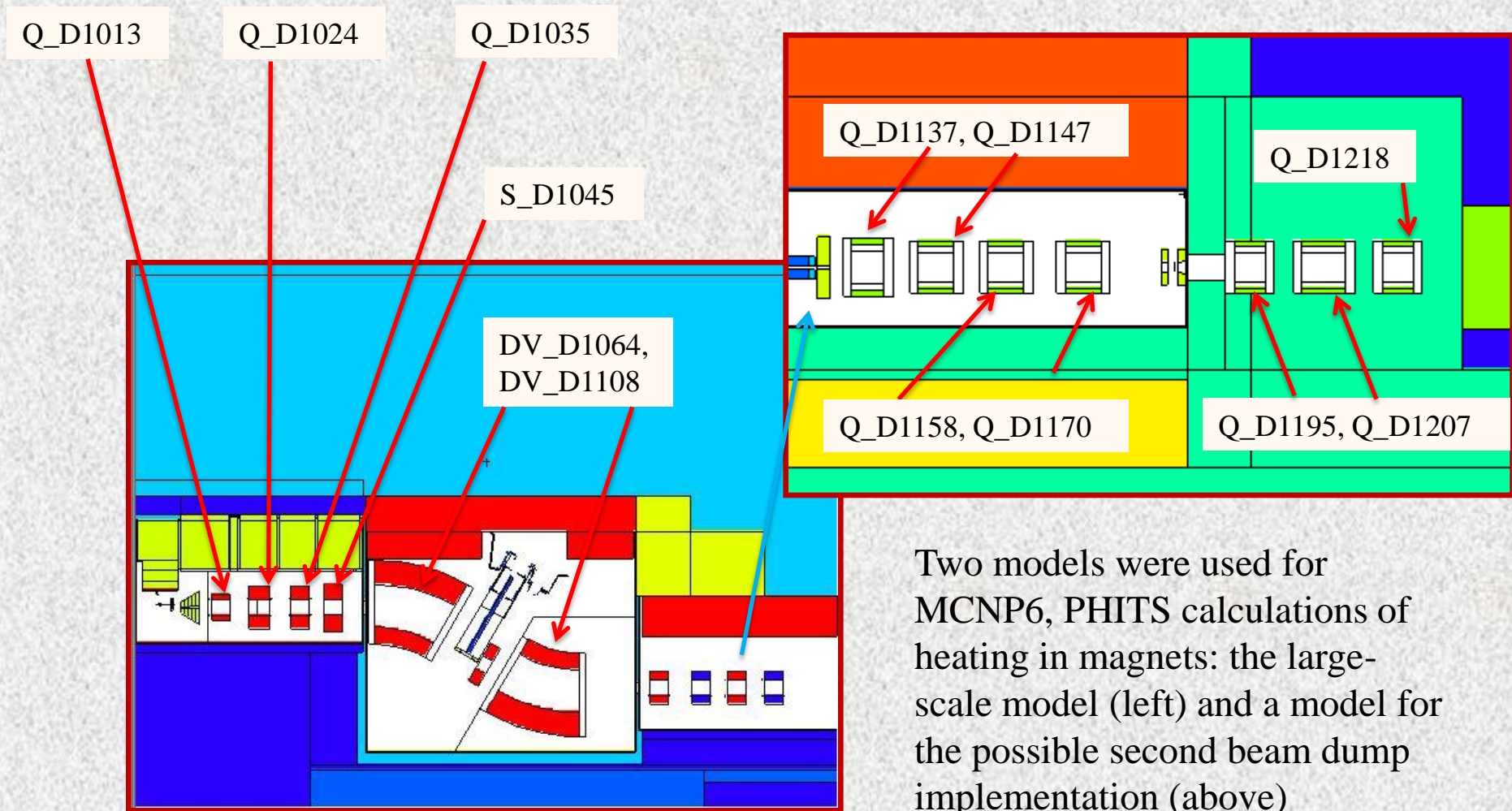
# Summary Table

Quantity\Model	LAQGSM+CEM, MIN f.	LAQGSM+CEM,MA X f.	Default, MIN
T. Neutron flux n/cm <sup>2</sup> /s	8.5E9	8.3E9	7.9E9
HE Neutron flux n/cm <sup>2</sup> /s	3.1E9	3.0E9	2.4E9
Power density, uW/g	16	17	9
DPA, /yr	3.1E-5	3.2E-5	2.4E-5
Absorbed dose, kGy/yr	330	330	170





# Radiation Heating in Magnets Determined Supports Magnet and Non-conventional Utility Design



# Expected Life of Preseparator Magnets

Iron, W shields studied

Need to value-engineer shield

Average heating quoted, maximum values under study and are likely factors of several larger

	Iron Shield					W Shield				
Projectiles	O18	Ca48	Kr86	Xe136	U238	O18	Ca48	Kr86	Xe136	U238
Energy (Mev/nucleon)	266	239.5	233	222	203	266	239.5	233	222	203
	Expected Life [y]					Expected Life [y]				
Q1b (BDS)	1.7E+04	3.3E+04	6.3E+04	6.9E+04	9.0E+04		1.63E+04	2.72E+04	4.55E+04	4.55E+04
Q2b (BDS)										
Q3b (BDS)	3448	6784	11765	14493	19011		3401	5675	9452	5675
Q_D1013	2	4	5	68	6		9	15	32	6
Q_D1024	149	368	391	481	435		397	1323	2415	2778
Q_D1035	66	80	130	495	179		242	180	120	17
OCT_D1045	1818	1946	7364	495	4630		7003	11820	16077	14205
DV_1064	37	28	45	561	36		28	42	96	35
S_D1092	71	79	5	78	5		80	7	391	5
DV_D1108	3333	3731	706	867	2688		284	370	318	407
Q_D1137	2500	13228	994	2907	3067		2463	26178	25126	8532
Q_D1147	1333	2404	216	39	6570		16722	16835	3086	1381
Q_D1158	1333	7062	7645	72	21930		92593	6196	30	329
Q_D1170	1048	30303	862	110	21645		45045	5675	12690	2841



# Displacements Per Atom (DPA)

- To evaluate radiation damage, a fundamental parameter that characterizes lattice displacement events is required.
- Dpa has been used to compare radiation damage by different radiation sources. It is a damage-based exposure unit and represents the number of atoms displaced from their normal lattice sites as a result of energetic particle bombardment.
- Calculations of dpa values

$$N_d = \begin{cases} \frac{\kappa(T - E_e)}{2E_d} = \frac{\kappa T_{dam}}{2E_d}, & T_{dam} > 2E_d \\ 1, & E_d < T_{dam} < 2E_d \\ 0, & 0 < T_{dam} < E_d \end{cases}$$

$$dpa = \Phi \sigma = \Phi \int_{E_d}^{T_{max}} \frac{d\sigma(E, T)}{dT} N_d$$

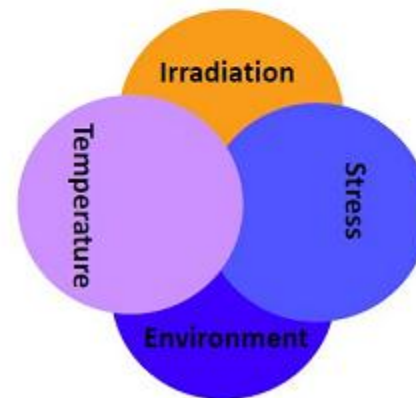
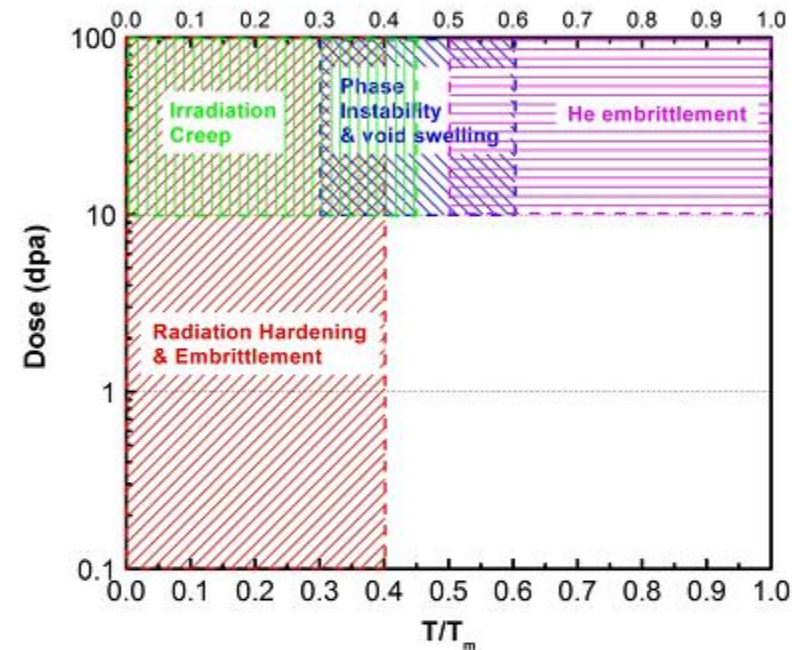
- $N_d$  is the number of displaced atoms produced by a PKA
- $T$  is the recoil energy of a PKA;  $E_e$  is the total energy lost by electron excitation;  $k$  is the damage efficiency;  $T_{dam}$  is the damage energy available for elastic collisions; and  $E_d$  is the threshold displacement energy.  $\sigma(E)$  is the displacement cross section for an incident particle at an energy  $E$ .

- Irradiation-induced changes of material properties are measured as a function of dpa



# Radiation-induced Property Changes

- Radiation-induced microstructural changes significantly degrade materials' properties
  - Degradation of physical properties (increase in electrical resistivity, decrease in thermal conductivity, etc.)
  - Radiation hardening and embrittlement
  - Irradiation creep
  - Void swelling
  - High temperature He embrittlement
  - Reduction in fatigue performance, irradiation-assisted stress corrosion cracking
- Synergistic effects of radiation, corrosive media, temperature, and stress





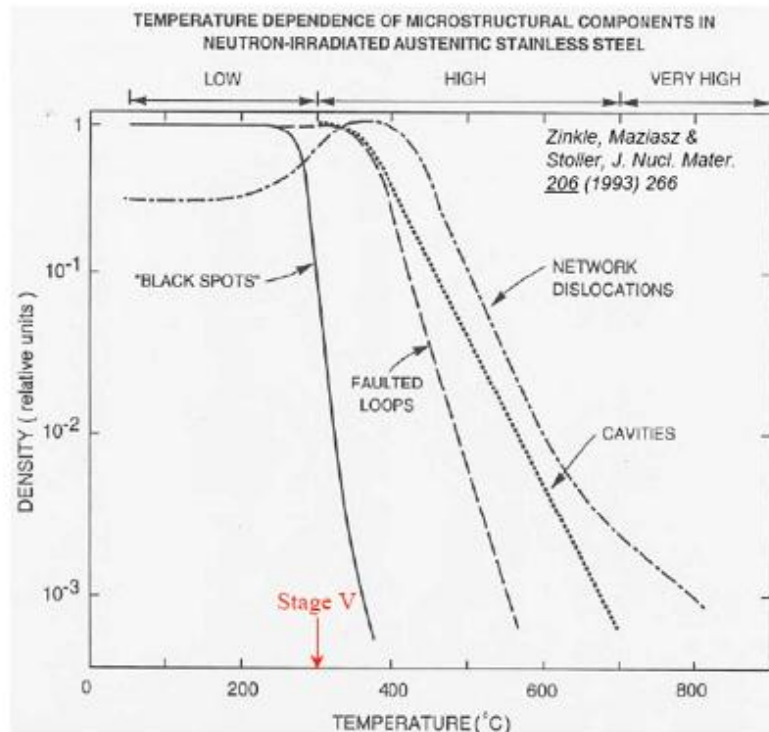
# Damage Correlation

- Dpa is a most commonly-used damage correlation parameter. However, damage correlation and data extrapolation must consider other aspects and base on a fundamental understanding
- Damage correlation parameters
  - Irradiation particle type, energy
  - Energy spectra
  - Flux or dose rate (dpa/s)
  - Fluence or dose (dpa)
  - Irradiation temperature
  - Transmutation (e.g. He, H)
  - Pulsed irradiation vs. continuous irradiation

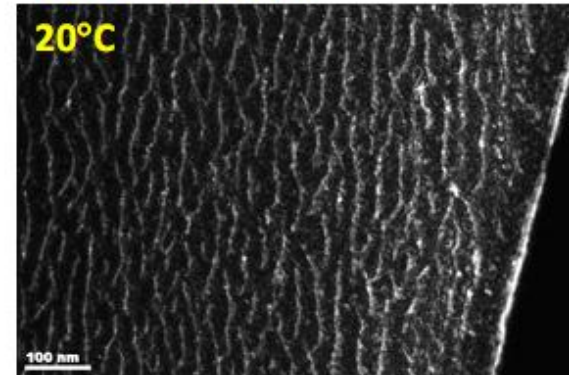


# Effect of Irradiation Temperature

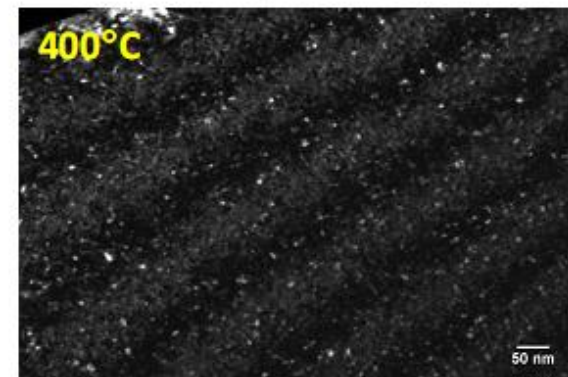
- Irradiation at different temperatures can result in different defect structures



Dose = 0.64 dpa



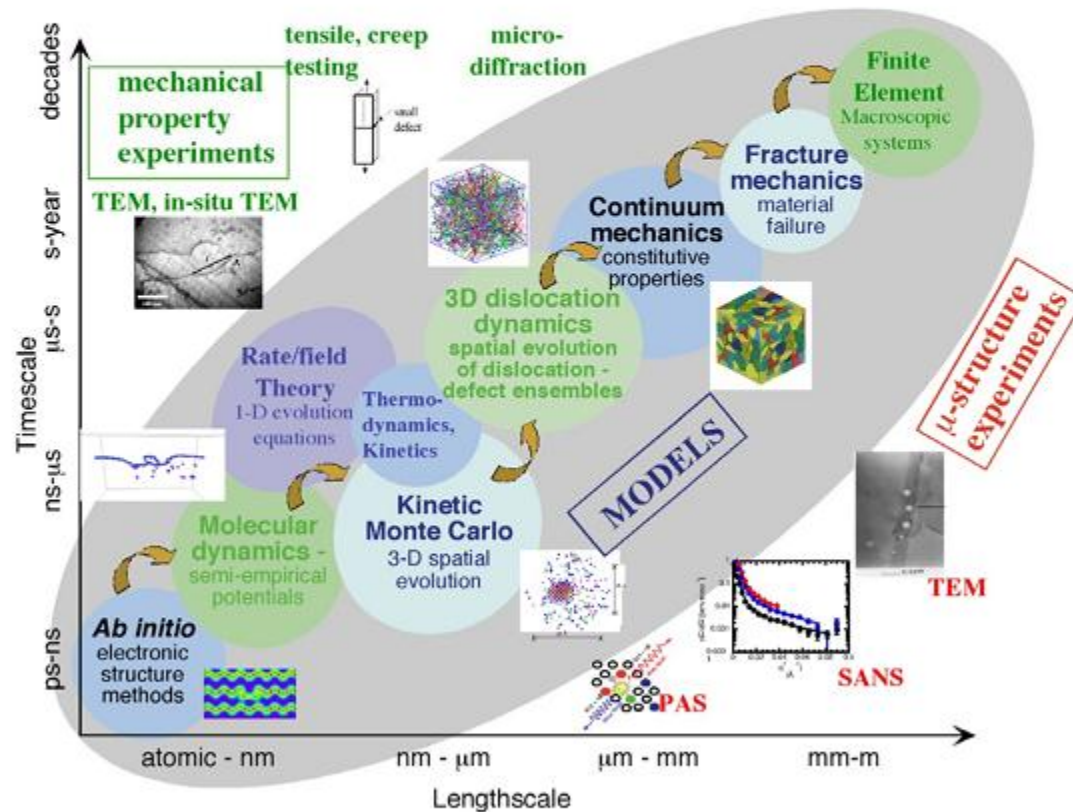
Dose = 0.64 dpa





# Radiation Modeling and Benchmark Experiments

- Effective radiation damage correlation requires close coordination between experimental, theoretical and computational studies.

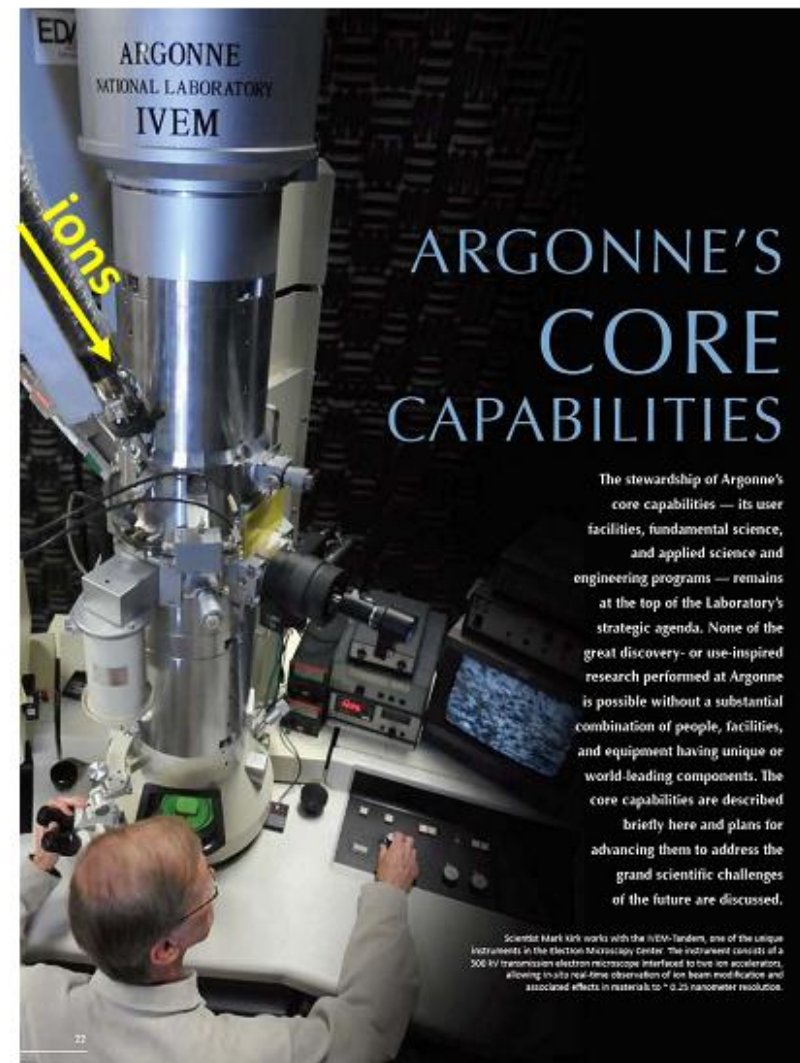


B. Wirth et al (2004)



# Ion Irradiation and Implantation

- *In situ* TEM ion irradiation is a powerful tool for introducing disorders in materials and validate and verify computer models
  - Real-time observation of defect formation and evolution during irradiation
  - A wide range of techniques including imaging, electron diffraction, and spectroscopy
  - Well-controlled conditions (temperature, ion, ion energy, dose rate, dose)
  - High doses (e.g. 100 dpa) can be achieved in hours; irradiation dose rates can be varied over several orders of magnitude
  - Studies of single-parameter effects and synergistic effects of irradiation, temperature and stress



## ARGONNE'S CORE CAPABILITIES

The stewardship of Argonne's core capabilities — its user facilities, fundamental science, and applied science and engineering programs — remains at the top of the Laboratory's strategic agenda. None of the great discovery- or use-inspired research performed at Argonne is possible without a substantial combination of people, facilities, and equipment having unique or world-leading components. The core capabilities are described briefly here and plans for advancing them to address the grand scientific challenges of the future are discussed.

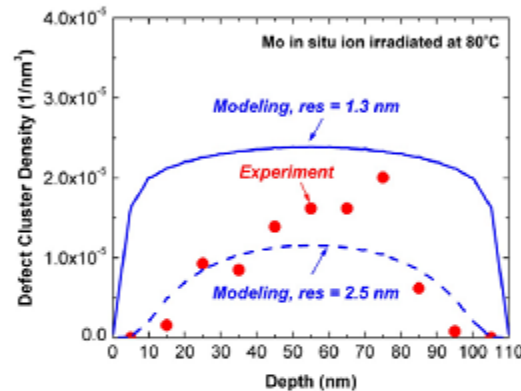
Scientist Mark Kirk works with the IVEM-Tandem, one of the unique instruments in the Electron Microscopy Center. The instrument consists of a 300 kV transmission electron microscope interfaced to have ion accelerators, allowing in-situ real-time observation of ion beam modification and associated effects in materials to ~0.25 nanometer resolution.

**IVEM:** Hitachi H-9000NAR, 100-300 kV, 0.2-1000 kx, spatial res 0.25 nm, time res 0.03 sec,  
**Irradiation:** All ions, 1 MeV max.  
**Loading:** 20 – 1273 K, straining stage



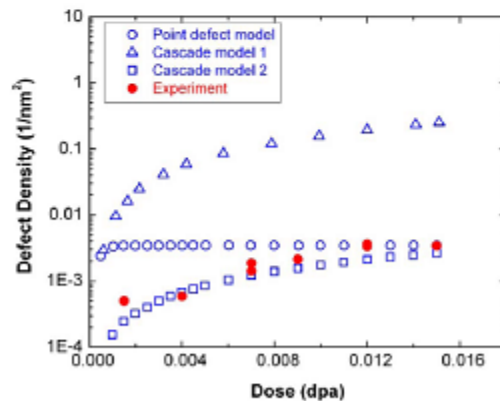
# Direct Comparison

- Quantitative, absolute comparisons between experiments and modeling at the same spatial and time scales is leading to the establishment of an accurate, reliable computer model.



- The spatially-dependent cluster dynamics model captured the essential physics of damage in irradiated Mo thin films.*

- Iterative refinement of key material parameters with in situ ion irradiation data led to a more accurate cluster dynamic model.*



## Conclusions

1. Substantial progress over last few years with Monte-Carlo codes used in this field; in majority of cases integral values on particle yields, energy deposition and radiation field can be predicted with accuracy of  $< 10\%$ .
2. Uncertainties of a factor of 2 or more still remain for differential values in some phase space regions as well as for values of DPA.
3. Data needs are identified for each class.
4. Comprehensive studies are performed on Mu2e, COMET, FRIB and Muon Collider.
5. Powerful tools, amazing results and their benchmarking were presented on radiation effects in nano-electronics; synergy and mutual interest in collaboration.
6. Moving from DPA to changes in materials: damage correlations; first direct benchmarking of DPA (MD model).